

Isopropanol-d7
19214-96-1 | DTXSID50480717

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 5.72×10^{-12} cm³/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 7.36×10^{-1}

Confidence level: 6.66×10^{-1}

Nearest Neighbors from the Training Set

Image not found

Isopropanol

Measured: 5.07×10^{-12}

Predicted: 5.72×10^{-12}

Image not found

1-Propanol

Measured: 5.53×10^{-12}

Predicted: 7.35×10^{-12}

Image not found

1,4-Diazabicyclo[2.2.2]octane

Measured: 2.20×10^{-11}

Predicted: 1.30×10^{-11}

Image not found

Diethyl ether

Measured: 1.31×10^{-11}

Predicted: 9.74×10^{-12}

Image not found

tert-Butyl alcohol

Measured: 1.12×10^{-12}

Predicted: 3.20×10^{-12}